2,2-Dimethylpentanedioic acid 681-57-2 | DTXSID6021585

001-37-2	D1721D0051202

Model Performance

N.A. I. I.	D .
Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (75%) Training (75%)		75%)	Test (25%)			
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 317 °C

Global applicability domain: Outside

Local applicability domain index: 6.24e-01

Confidence level: 5.44e-01

Nearest Neighbors from the Training Set

Image not found

Heptanedioic acid Measured: 342 Predicted: 332

Image not found

3-Ethyl-3-methylglutaric acid

Measured: 261 Predicted: 286

Image not found

Hexanedioic acid Measured: 338 Predicted: 330

Image not found

Octanedioic acid Measured: 346 Predicted: 332

Image not found

Pentanedioic acid Measured: 303 Predicted: 310